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13. ABSTRACT *(Maximum 200 words)*

Research on algorithms, strategies and problems associated with the numerical modeling of high frequency piezoelectric resonators was performed. The research was applied principally to SC-cut quartz crystal resonators vibrating at the third overtone of thickness shear mode and to piezoelectric laminated plates vibrating at the fundamental thickness shear mode. Finite elements using high frequency piezoelectric plate equations of motion were implemented in computer codes. Scientific visualization techniques of high frequency modes of vibration were performed. Algorithms for efficient storage of mass and piezoelectric stiffness matrices were proposed. Algorithms for the calculation of eigenpairs in the piezoelectric eigenvalue matrix problem were proposed. These algorithms reduced the memory requirement and computational time for large scale piezoelectric eigenvalue matrix problem by approximately two orders of magnitude over the current methods where the electrical degrees of freedom were separated from the mechanical degrees of freedom in the global piezoelectric stiffness matrix. The proposed method interleaved the electrical and mechanical degrees of freedom.

14. SUBJECT TERMS
Numerical modeling of high frequency piezoelectric resonators; visualization of high frequency modes of vibration; numerical algorithms for efficient storage of the mass, and piezoelectric stiffness matrices; reduction of computational time in large scale piezoelectric eigenvalue problem.

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Numerical Analysis of Third Harmonic Overtone of Thickness-Shear Vibrations in SC-Cut Quartz Resonators.

FINAL REPORT

Yook-Kong Yong

March 15, 1995

U. S. ARMY RESEARCH OFFICE
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Numerical Analysis of Third Harmonic Overtone of Thickness-Shear Vibrations in SC-Cut Quartz Resonators.

Final Report

Yook-Kong Yong
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I. Statement of the problem studied.

Research and development of numerical methods and visualization techniques for the analysis high frequency SC-cut quartz resonators vibrating at the third harmonic overtone of thickness-shear mode.

II. Summary of most important results.

1. Detailed numerical modeling and visualization of high frequency modes of vibration in quartz crystal resonators such as that of the fundamental thickness shear mode and its harmonic overtones were implemented. Software and hardwares for visualization of very high frequency plate vibrations were investigated. Visualization techniques for 2-D, 2.5-D and 3-D data sets were explored. The development and results were reported in publications 1 to 5.
2. Theoretical study and development of two-dimensional piezoelectric plate equations for the numerical modeling of very high frequency piezoelectric crystal resonators were completed. Dispersion curves for an infinite piezoelectric plate with free surfaces were calculated using both the three-dimensional piezoelectric equations, and the two-dimensional piezoelectric plate equations, and compared. The dispersion curves were calculated up to the third overtone of thickness shear. A good fit between the dispersion relations obtained from the two-dimensional piezoelectric plate equations and the three-dimensional theory indicates that the two-dimensional equations will yield accurate results. The comparison showed a relatively good fit for the real wave numbers which represented the propagating modes. The fit for the imaginary wave numbers which represented the evanescent modes were not as good. The third overtone SC-cut quartz resonator will vibrate in the vicinity of a normalized frequency equal to 2.8. Straight crested wave studies of SC-cut quartz plate resonators vibrating at the third harmonic overtone of thickness-shear mode were completed. The plate model incorporated all mechanical displacement and electric potential components up to the third order of Lee, Syngellakis and Hou's piezoelectric plate equations. Hence, there were 12 mechanical displacement components, and four electric potential components. The mass and electrical effects of a pair of electrode conducting films on the top and

bottom surfaces of the plate resonator were studied. The use of Muller's method in the calculation of the dispersion relations is critical if there were more than six components of displacements in the plate model. The results were reported in publication 7.

3. Finite element implementation of the piezoelectric plate equations and numerical modeling of SC-cut quartz resonators vibrating at the third overtone of thickness shear mode were performed. The results were reported in publications 8 and 13.

4. From our working experience on the finite element modeling of high frequency SC-cut quartz resonators, we learned some important strategies and problems in such numerical models:

   (a) For accurate representation of eigenpairs, the number of elements per half wave of eigenmode must be at least three or more.

   (b) The Lanczos algorithm for the eigenvalue problem was found to be superior in terms of accuracy and computational speed. The algorithm allowed for the calculation for a few eigenpairs in a narrow bandwidth at any frequency.

   (b) For the piezoelectric eigenvalue matrix problem, better algorithms were needed for managing storage memory and increasing computational speed. This was the motivation for the next phase of research.

5. Research on new algorithms for the solution of the piezoelectric eigenvalue matrix problem were performed. The customary method was to statically condense the dielectric matrix since the problem is electrostatic. The static condensation however destroyed the sparse matrix structure of the stiffness matrix, and caused unacceptable increase in memory storage and computational time. Two schemes were proposed:

   (a) A perturbation scheme in which the mechanical eigenvalue problem was solved independently and the piezoelectric effects were subsequently added as a perturbation. This scheme was however applicable only to materials with very weak piezoelectric coupling such as quartz. It would not be applicable to materials such as lithium niobate, zinc oxide, and aluminum nitride. The results were reported in publication 10. A new method for storing the mass matrix which reduced the memory storage by about 94% was also presented

   (b) A scheme which avoided static condensation of the dielectric matrix was implemented. This scheme was superior to the perturbation scheme because it was applicable to all piezoelectric materials, was simpler conceptually, and was more efficient in terms of memory and computational speed. The old customary scheme of storing the electrical degrees of freedom separate from the mechanical degrees of freedom was discarded. A new storage scheme which mixed the mechanical and electrical degrees of freedom in the global matrix so as to reduce its half-bandwidth was implemented. This resulted in savings of more than two orders of

magnitude in memory and computational speed. Part of the results were reported in publication 14. Further results will be reported in the Proceedings of the IEEE 1995 Ultrasonics Symposium.

6. Implementation of the finite element method for piezoelectric laminated plate with electrodes was performed. The studies were reported in publications 6, 9, 11, 12 and 15.
7. The accuracy of plate equations for straight crested waves at frequencies in the vicinity of the fundamental thickness shear mode in an SC-cut quartz strip. was examined. The first order plate theories with correction factors were currently assumed to predict accurately the plate modes of vibration at frequencies up to twenty percent higher than the fundamental thickness shear frequency. These plate equations were derived using a series expansion of the thickness modes with various functions of the thickness coordinate: (1) Power series (Mindlin), (2) trigonometric series (Lee, et. al.), (3) Legendre series (Mindlin, et. al.) and (4) normal modes (Peach). Our results showed that the first order plate equations did not yield accurate frequency spectra of the modes in the vicinity of the fundamental thickness shear mode, although the thickness shear mode itself was predicted accurately. Four finite element programs were used in the study. The programs individually calculated the straight crested wave frequency spectra as a function of the length to thickness ratio for an SC-cut quartz strip using (1) the first order Mindlin plate equations, (2) the third order Mindlin plate equations, (3) the third order Lee, et. al. plate equations, and (4) the three dimensional elastic equations. The numerical solutions for the three dimensional elastic equations were checked against the simple analytical solutions for an elastic membrane. The results showed that all the plate theories predicted the fundamental thickness mode accurately, but the frequency spectra of modes in the vicinity are not predicted well by the first order Mindlin plate equations and the third order Lee et. al. plate equations. The third order Mindlin plate equations, on the other hand, predicted very well the entire frequency spectrum in the vicinity. Hence, if an accurate prediction of the unwanted modes near the fundamental thickness shear mode was needed, the third order Mindlin plate equations were recommended. The third order Mindlin plate equations did not require shear corrections factors. The mode shapes of the third order displacement components showed a surprisingly large contribution to the resonant modes in the neighborhood of the fundamental thickness shear frequency. The results will be reported in the Proceedings of the IEEE 1995 Annual Symposium on Frequency Control.

III. Interactions with the U.S. Army Research Laboratory, Electronics & Power Sources Directorate, Fort Monmouth.

Interactions are maintained with Dr. Arthur Ballato and Dr. John R. Vig of the U.S. Army Research Laboratory, Electronics & Power Sources Directorate, Fort Monmouth. There are current works on acceleration sensitivity of SC-cut quartz crystal resonators at the said laboratory. Numerical modeling and visualization of very high frequency quartz crystal resonators can be applied to acceleration sensitivity studies.

IV. List of publications

1. "Thickness Shear Mode Shapes and Mass Frequency Influence Surface of a Circular and Electroded AT-Cut Quartz Resonator," J.T. Stewart and Y-K. Yong, Applications of Supercomputers in Engineering II, Editors: C.A. Brebbia, D. Howard and A. Peters, Elsevier Applied Science, New York, 1991, pp 513-527.

2. "Thickness Shear Mode Shapes and Mass Frequency Influence Surface of a Circular and Electroded AT-Cut Quartz Resonator," Y-K. Yong, J.T. Stewart, J. Detaint, A. Zarka, N. Capelle and Y. Zheng, Proceedings of the 45th Annual Symposium on Frequency Control, 1991, pp 137-147.

3. "Visualization Techniques for Bulk Wave Resonators," D. Silver, J.T. Stewart and Y-K. Yong, Proceedings of the IEEE 1991 Ultrasonics Symposium, 1991, pp 499-504.

4. "Mass Frequency Influence Surface, Mode Shapes, and Frequency Spectrum of a Rectangular AT-Cut Quartz Plate," Y-K. Yong and J.T. Stewart, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. UFFC-38, No.1, January 1991, pp 67-73.

5. "Thickness Shear Mode Shapes and Mass Frequency Influence Surface of a Circular and Electroded AT-Cut Quartz Resonator," Y-K. Yong, J.T. Stewart, J. Detaint, A. Zarka, B. Capelle and Y. Zheng, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. UFFC-39, No.5, September 1992, pp 609-617.

6. "Piezoelectric, Laminated Composite Plate Theory for Thin Film Resonators," Y-K. Yong and J.T. Stewart, Proceedings of the IEEE 1991 Ultrasonics Symposium, 1991, pp 517-522.

7. "On Straight Crested Waves in a Third Overtone SC-Cut Quartz Resonator," Y-K. Yong and Z. Zhang, Proceedings of the 1992 IEEE Frequency Control Symposium, 1992, pp. 567-581.

8. "Numerical Algorithms and Results for a SC-Cut Quartz Plate Vibrating at the Third Harmonic Overtone of Thickness Shear," Y-K. Yong and Z. Zhang, Proceedings of the IEEE 1993 Ultrasonics Symposium, 1993, pp. 553-558.

9. "Exact Analysis of the Propagation of Acoustic Waves in Multilayered Anisotropic Piezoelectric Plates," J.T. Stewart and Y-K. Yong, Proceedings of the 1993 IEEE Frequency Control Symposium, 1993, pp. 476-501.

10. "A Perturbation Method for Finite Element Modeling of Piezoelectric Vibrations in Quartz Plate Resonators," Y-K Yong and Z. Zhang, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 40, No. 5, September 1993, pp 551-562.

11. "A Laminated Plate Theory for High Frequency, Piezoelectric Thin-Film Resonators," Y-K Yong, J.T. Stewart, and A. Ballato, Journal of Applied Physics, Vol. 74, No. 5, September, 1993, pp 3028-3046.

12. "Exact Analysis of the Propagation of Acoustic Waves in Multilayered Anisotropic Piezoelectric Plates," J.T. Stewart, and Y-K Yong, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 41, No. 3, May 1994, pp 375-390.

13. "Numerical Algorithms and Results for SC-Cut Quartz Plates Vibrating at the Third Harmonic Overtone of Thickness Shear," Y-K Yong and Z. Zhang, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, Vol. 41, No. 5, September, 1994, pp 685-693.

14. "Algorithms for Eigenvalue Problems in Piezoelectric Finite Element Analyses," Y. Cho and Y-K Yong, Proceedings of the IEEE 1994 Ultrasonics Symposium, 1994, pp 1057-1062.

15. "Numerical Analysis of Thickness Shear Thin Film Piezoelectric Resonators Using a Laminated Plate Theory," Z. Zhang and Y-K Yong, IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control, (Accepted for publication.)

16. "Exact and Approximate Analysis of the Propagation of Acoustic Waves in Layered Piezoelectric Plates," James T. Stewart, Ph. D. thesis, 1993, Dept. of Civil and Environmental Engineering, Rutgers, the State University of New Jersey.

17. "Numerical Analysis of the Third Overtone of Thickness Shear Vibrations in SC-Cut Quartz Resonators," Zhen Zhang, Ph. D. thesis, 1993, Dept. of Civil and Environmental Engineering, Rutgers, the State University of New Jersey.

V. List of Participating Personnel

1. James T. Stewart, Ph.D., Rutgers, the State University of New Jersey, 1993
2. Zhen Zhang, Ph.D., Rutgers, the State University of New Jersey, 1994

APPENDIX

Abstracts of most important publications.

Visualization Techniques for Bulk Wave Resonators

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Abstract

In this paper, we present an overview of some fundamental algorithms for visualizing multi-dimensional data sets. These techniques are applied to ongoing research problems in bulk wave piezoelectric resonators.

Introduction

The goal of large scale simulations and experiments in computational science is a quantitative and mathematical understanding of the model being investigated. A key component in this process is visualization: the use of computer graphics to depict and project the resulting data. As experiments become more sophisticated, the data generated becomes overwhelming and new techniques are needed to help understand and aid in its interpretation.

The sequence of steps involved in this process can be summarized as follows:

- Data generation (simulation, etc.)
- Filtering, i.e. deriving other variables, interpolation, etc.
- Creating geometric primitives: converting the data to a form suitable for rendering.
- Rendering: Displaying the geometry (with shading, transparency...)

This is process is not a static one, i.e. the process may involve many iterations before a *suitable* visualization results.

Scientific visualization is an active and growing field. Almost all domains of science are incorporating computer graphics algorithms into standard scientific experiments. These fields include computational fluid dynamics, medical imaging, molecular biology, chemistry, meteorology, etc. Although each scientific domain has specific requirements, most of the procedures used are generic and can be adapted to other fields. Now that finite element solutions (2D and 3D) are more common for bulk wave resonators, visualization techniques are becoming increasingly important to help in the analysis of the resulting data sets.

In this paper, we present an overview and implementation details of some fundamental algorithms for visualizing multi-dimensional data sets. These techniques are applied to ongoing research problems in bulk wave piezoelectric resonators. These methods may be useful for

- Identifying modes: for example, thickness shear, overtones (Figure 2), and energy trapping phenomena (Figure 3);
- Detecting symmetry: whether a mode is symmetric or anti-symmetric (Figure 13);
- Determining mounting strategies: locate zero-values (Figure 7).

In the first section, we present a set of two dimensional routines. For modeling a vibrating resonator using 3D finite elements, a combination of slicing, isosurface contours, and volume visualization are used. These techniques are also applicable to layer-wise plate theory. We hope to show that using visualization tools can greatly enhance the process of scientific discovery and progress in this area of research.

(Note: The pictures presented in this paper were originally in color - some of the effects, especially transparency, do not reproduce well in black and white.)

Two Dimensional Techniques

This section discusses methods for visualizing 2D scalar fields (i.e. an x,y grid with a value at each node) resulting from finite element solutions for the

Mass-Frequency Influence Surface, Mode Shapes, and Frequency Spectrum of a Rectangular *AT*-Cut Quartz Plate

Yook-Kong Yong, *Member, IEEE* and James T. Stewart

Abstract—The mass-frequency influence surface and frequency spectrum of a rectangular *AT*-cut quartz plate is studied. The mass-frequency influence surface is defined as a surface giving the frequency change due to a small localized mass applied on the plate surface. Finite-element solutions of Mindlin's two-dimensional (2-D) plate equations for thickness-shear, thickness-twist, and flexural vibrations are given. Spectrum splicing, and an efficient eigenvalue solver using the Lanczos algorithm were incorporated into the finite-element program. A convergence study of the fundamental thickness-shear mode and its first symmetric, anharmonic overtone was performed for finite-element meshes of increasing fineness. As a general rule, more than two elements must span any half-wave in the plate or spurious mode shapes will be obtained. Two-dimensional (2-D) mode shapes and frequency spectrum of a rectangular *AT*-cut plate in the region of the fundamental thickness-shear frequency are presented. The mass-frequency influence surface for a 5-MHz rectangular, *AT*-cut plate with patch electrodes is obtained by calculating the frequency change due to a small mass layer moving over the plate surface. The frequency change is proportional to the ratio of mass loading to mass of plate per unit area, and is confined mostly within the electrode area, where the magnitude is of the order 10^8 Hz/g.

I. Introduction

The primary effect of mass loading on a thickness-shear resonator is well known, that is, the resonator frequency is lowered in proportion to the magnitude of mass loading. It was shown theoretically [1], [2] that very small, fluctuating mass loading, namely that of a fluctuating monolayer of molecules, can have a measurable effect on the phase fluctuations of ultra-high-frequency resonators. In this paper, the frequency effect of small mass loadings on a 5-MHz, rectangular *AT*-cut quartz plate with rectangular electrode films is calculated using finite element solutions of Mindlin's plate equations with mass loadings [3]. The plate resonator is vibrating in the fundamental thickness-shear mode. The frequency spectrum and mode shapes of resonant modes in the region of the fundamental thickness-shear mode are also presented.

II. Mindlin's Plate Equations for Thickness-Shear, Thickness-Twist, and Flexural Vibrations in an *AT*-Cut, Electrode Plated Quartz Plate

The calculation of frequency change due to a small, discrete mass loading on a plate surface lends itself naturally to the finite element method. Mindlin's equations for an *AT*-cut, electrode plated quartz plate [3], [4] are employed. Lee, Zee, and Brebbia [5] employed these equations in their study of the influence of the size and mass of rectangular patch electrodes on the vibrations and energy trapping in a rectangular *AT*-cut quartz plate. Fig. 1 shows a rectangular crystal plate of density ρ, thickness 2b, length 2l, and width 2w that is partially plated on the top and bottom surfaces by electrode platings of density ρ', thickness $2b'$, length 2a, and width 2c over the central portion of its faces.

A. Stress Equations of Motion

The stress equations of motion accommodating thickness-shear, thickness-twist, and flexural vibrations are

$$Q_{1,1} + Q_{3,3} = 2b\rho(1 + R)\ddot{u}_2, \tag{1}$$

$$M_{1,1} + M_{5,3} - Q_1 = \tfrac{2}{3} b^3\rho(1 + 3R)\ddot{\psi}_1, \tag{2}$$

$$M_{5,1} + M_{3,3} - Q_3 = \tfrac{2}{3} b^3\rho(1 + 3R)\ddot{\psi}_3, \tag{3}$$

where the terms Q_i ($i = 1, 3$) are the transverse shear forces per unit length, and M_i, for $i = 1$, or 3, are the bending moments per unit length, and, M_5 is the twisting moment per unit length. The term $R = 2\rho' b'/(\rho b)$ is ratio of mass of electrodes to mass of plate per unit area. Displacement u_2 is the transverse displacement in the x_2 direction, and ψ_1, and ψ_3 are shear rotations about the x_1, and x_3 axes, respectively.

B. Stress-Strain Relations

For an *AT*-cut quartz plate, the elastic constants exhibits monoclinic symmetry when the x_1 axis coincides with one of the digonal axes of crystal. The constitutive relations are

$$Q_1 = 2b\bar{k}_1^2 C_{66}\gamma_1 \tag{4}$$

$$Q_3 = 2b\bar{k}_3^2 \overline{C}_{44}\gamma_3 \tag{5}$$

$$M_1 = \tfrac{2}{3}b^3(\hat{C}_{11}\chi_1 + \hat{C}_{13}\chi_3) \tag{6}$$

$$M_3 = \tfrac{2}{3}b^3(\hat{C}_{13}\chi_1 + \hat{C}_{33}\chi_3) \tag{7}$$

and

$$M_5 = \tfrac{2}{3}b^3\hat{C}_{55}\chi_5 \tag{8}$$

where γ_i ($i = 1, 3$) are the shear strains, and χ_1, χ_3, and χ_5 are the x_1 bending curvature, x_3 bending curvature, and twisting curvature, respectively. The coefficients $\bar{k}_1^2$ and $\bar{k}_3^2$ in (4) and (5) are shear correction factors that include mass loading effects

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IEEE Log Number 9040250.

Thickness-Shear Mode Shapes and Mass-Frequency Influence Surface of a Circular and Electroded *AT*-Cut Quartz Resonator

Yong-Kong Yong, *Member, IEEE*, James T. Stewart, Jacques Détaint, Albert Zarka, Bernard Capelle, and Yunlin Zheng

Abstract—**Finite-element solutions for the fundamental thickness shear mode and the second-anharmonic overtone of a circular, 1.87 MHz *AT*-cut quartz plate with no electrodes are presented and compared with previously obtained results for a rectangular plate of similar properties. The edge flexural mode in circular plates, a vibration mode not seen in the rectangular plate, is also presented. A 5-MHz circular and electroded *AT*-cut quartz plates is studied. A portion of the frequency spectrum is constructed in the neighborhood of the fundamental thickness-shear mode. A convergence study is also presented for the electroded 5-MHz plate. A new two-dimensional (2-D) technique for visualizing the vibration mode solutions is presented. This method departs substantially from the three-dimensional (3-D) "wire-frame" plots presented in the previous analysis. The 2-D images can be manipulated to produce nodal line diagrams and can be color coded to illustrate mode shapes and energy trapping phenomenon. A contour plot of the mass-frequency influence surface for the plated 5-MHz resonator is presented. The mass-frequency influence surface is defined as a surface giving the frequency change due to a small localized mass applied to the resonator surface.**

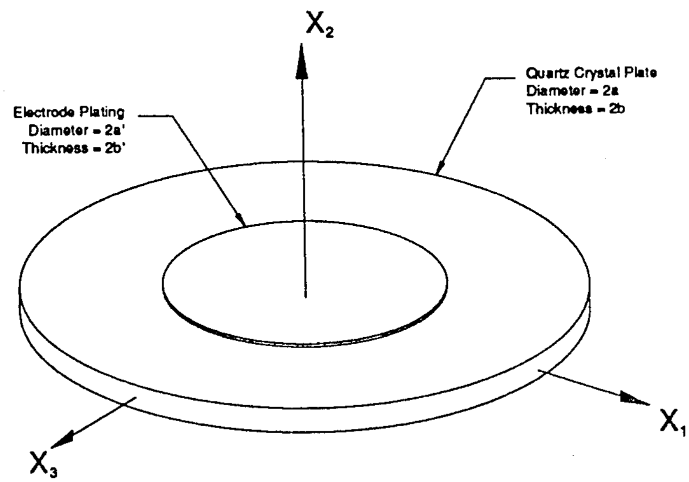

Fig. 1. Orientation and dimensions of a circular electroded plate.

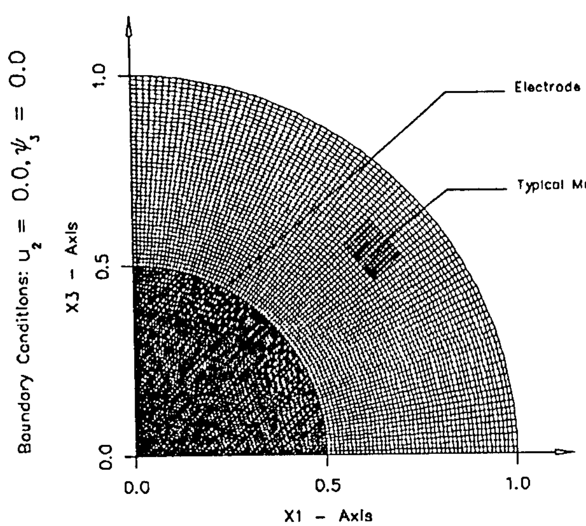

Fig. 2. Finite-element mesh of quarter circular plate with essential boundary conditions at the plate edges along the coordinate axes.

I. Introduction

The use of quartz crystal plates in ultrasonics is well studied experimentally. Analytical closed form solutions of a freely vibrating anisotropic elastic plate can in general only be obtained for either a one-dimensional (1-D) problem, or in an infinite domain. For a two-dimensional (2-D) finite domain, solutions may be obtained either approximately, or for certain specific types of boundary conditions and geometries. To perform a practical analysis of the *AT*-cut quartz resonator, it is necessary to solve the free vibration problem for a finite plate. In this paper, such a problem is solved using the finite-element method.

The high frequency vibrations as well as the anisotropicity of quartz demands that a general thick plate theory be used. In this study, Mindlin's 2-D plate equations are truncated to a first-order approximation. The first-order approximation is chosen because it is the lowest-order formulation which includes the major modes of interest, namely, the fundamental thickness-shear modes [2]. Real *AT*-cut resonators generally contain a thin electrode plating on a portion of each face, across which a time varying voltage is applied to drive the vibration. The effect of this electrode plating was studied analytically by Mindlin [3] for an infinite plate. Mindlin's equations for the electroded plate are incorporated into the

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J. Detaint is with the CNET Department of the PAB/BAG/MCT/CMM, 196 rue de Paris, 92220 Bagneux, France.
A. Zarka, N. Capelle, and Y. Zheng are with the L.M.C. Université, Paris, France.

IEEE Log Number 9201918.

On Straight Crested Waves in a Third Overtone SC-Cut Quartz Resonator.

Y-K Yong and Z. Zhang

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Abstract

Finite element matrix equations employing high frequency, piezoelectric plate equations are derived. The equations may be used for modeling third harmonic overtone of thickness-shear vibrations. A perturbation technique is developed to account for piezoelectric stiffening in the mechanical stiffness matrix. Results from the perturbation method compares well with the direct solution of the piezoelectric finite element equations. The technique will result in significant savings in computer memory and computational time. Numerical results for straight crested waves in a third overtone SC-cut quartz strip with and without electrodes are presented. Steady state response to an electrical excitation is calculated.

I. Introduction

We discuss in this paper the finite element formulation and results on straight crested waves in the vicinity of the third harmonic overtone of thickness shear, piezoelectric vibrations in a SC-cut quartz strip. The straight crested waves are spatially one-dimensional, but since the study is part of a wider study of third overtone SC-cut quartz resonators, two-dimensional finite element equations for piezoelectric plate vibrations are derived and presented. A one-dimensional finite element program is developed which could be modified subsequently to handle two-dimensional problems. The mechanical stiffness of the finite element matrix equations for the SC-cut quartz strip is a few orders of magnitude larger than the piezoelectric stiffness, and the piezoelectric coupling is weak. Hence, the piezoelectric effects could be modelled using a perturbation technique. A new perturbation method for piezoelectric vibrations is derived and proposed.

II. Plate Equations for High Frequency Piezoelectric Vibrations.

The piezoelectric plate equations for high frequency vibrations employed in the current finite element formulation were derived by Lee, Syngellakis and Hou [1]. The components of mechanical displacement and electric potential are expanded in an infinite series with their thickness-dependence expressed by trigonometric functions:

$$\begin{aligned} u_i(x_1,x_2,x_3,t) &= \sum_{n=0}^{\infty} u_i^{(n)}(x_1,x_3,t)\cos\frac{n\pi}{2}(1-\xi) \\ \phi(x_1,x_2,x_3,t) &= \sum_{n=0}^{\infty} \phi^{(n)}(x_1,x_3,t)\cos\frac{n\pi}{2}(1-\xi) \end{aligned} \tag{1}$$

where $\xi = \frac{x_2}{b}$ is a nondimensional thickness coordinate of the plate. The terms $u_j^{(n)}$ and $\phi^{(n)}$ are functions of spatial coordinates x_1 and x_3 only and time t. We present without formal derivations the following field equations from reference [1]. The interested reader may obtain

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Numerical Algorithms and Results for SC-Cut Quartz Plates Vibrating at the Third Harmonic Overtone of Thickness Shear

Y.-K. Yong, *Member, IEEE* and Zhen Zhang

***Abstract*—Finite element matrix equations, derived from two-dimensional piezoelectric high frequency plate theory are solved to study the vibrational behavior of the third overtone of thickness shear in square and circular SC-cut quartz resonators. The mass-loading and electric effects of electrodes are included. A perturbation method which reduces the memory requirements and computational time significantly [2] is employed to calculate the piezoelectric resonant frequencies. A new storage scheme is introduced which reduces memory requirements for mass matrix by about 90% over that of the envelope storage scheme. Substructure techniques are used in eigenvalue calculation to save storage. Resonant frequency and the mode shapes of the harmonic third overtone thickness shear vibrations for square and circular plates are calculated. A predominant third overtone thickness shear displacement, coupled with the third overtone of thickness stretch and thickness twist, is observed. Weak coupling between the third order thickness shear displacement and the zeroth-, first-, and second-order displacements is noted. The magnitudes of the lower order displacements are found to be about two orders smaller than that of the third overtone thickness shear displacement.**

I. INTRODUCTION

THIS paper describes computational strategies in the finite element analysis of SC-cut quartz resonators, and presents the numerical results of the third overtone thickness shear modes in SC-cut quartz plates. Theoretical developments and applications of the high frequency piezoelectric plate equations were presented in [1] and [2], and would not be repeated here. The interested reader should refer to the two references for further details. One obstacle in the finite element modeling of high frequency plate vibrations is the limitation of computer memory. A finite element model using two-dimensional (2-D) piezoelectric plate equations provides an excellent approximation of the vibrational behavior of plate resonators, and at the same time requires less memory than the three-dimensional finite element model. The characteristics of a good finite element program rest on its memory saving strategies as well as its computational efficiency.

The finite element matrix equations are based on the piezoelectric plate theory derived by Lee, Syngellakis, and Hou [1]. The plate theory is chosen for its accuracy in predicting cutoff frequencies of harmonic overtones of thickness vibrations. Twelve mechanical displacement and four electric potential components, $u_j^{(n)}$ and $\phi^{(n)}$, ($j = 1,2,3$, and $n = 0,1,2,3$), are incorporated into the numerical model for the analysis of vibrations with frequencies in the vicinity of the harmonic third overtone thickness modes. The mass-loading and electric effects of platings are also included. In piezoelectric vibrations, the terms in the stiffness matrix consist of two parts, namely, the mechanical stiffness and piezoelectric coupling stiffness. The latter, even though it is a few orders of magnitude less than the mechanical terms for SC-cut quartz, destroys the sparse structure of the stiffness matrix. A perturbation method [2] is introduced to separately calculate the piezoelectric frequencies from the purely mechanical frequencies for quartz resonators.

In the calculations of purely mechanical frequencies, a new storage scheme for the mass matrix is developed which takes advantage of its special structure and reduces the memory requirements by about 90% over that of the envelope storage scheme during the Cholesky factorization, and a substructuring scheme is employed to further diminish the storage demands.

Resonant frequencies of the harmonic third overtone thickness shear and the associated mode shapes are calculated for rectangular and circular SC-cut quartz plate resonators. A clean third overtone thickness shear displacement, coupled with the third overtone of thickness stretch and thickness twist, is observed. The magnitudes of zeroth, first and second order displacement components are one to two orders smaller than those of the third-order displacement components.

II. NUMERICAL STRATEGIES FOR SC-CUT PLATES VIBRATING AT THE THIRD OVERTONE OF THICKNESS SHEAR

The finite element matrix equations for piezoelectric vibrations have the following form [2]:

$$K_0 d + P^T \psi + M\ddot{d} = F_S + F_C \tag{1}$$

$$Pd - R\psi = Q_S + Q_C \tag{2}$$

where matrices K_0, P, R, and M are, respectively, the element mechanical stiffness, piezoelectric coupling, dielectric stiffness, and mass. The vectors F_S, F_C, Q_S, and Q_C are element face traction, edge traction, face charge, and edge charge, respectively, [2]. The general piezoelectric eigenvalue equations (3) and (4) may be derived from (1) and (2) by setting the right-hand side vectors to zero and assuming the harmonic motion, namely, $d = \bar{d}e^{i\omega t}$ and $\psi = \bar{\psi}e^{i\omega t}$:

$$K_0\bar{d} + P^T\bar{\psi} = \omega^2 M\bar{d} \tag{3}$$

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Exact Analysis of the Propagation of Acoustic Waves in Multilayered Anisotropic Piezoelectric Plates

James T. Stewart and Yook-Kong Yong, *Member, IEEE*

***Abstract*—Exact analysis of the propagation of acoustic waves in multilayered piezoelectric plates is performed using the transfer matrix method. A general technique for analyzing layered piezoelectric resonators under thickness and lateral field excitation is presented and is applied to the study of zinc oxide on silicon thin film resonators. Both one and two-dimensional analysis with general material anisotropy is performed, and a simplified method for incorporating thin conducting electrodes on the plate's free surfaces is presented. The general methodology described is summarized into efficient algorithms to aid in the implementation of the procedures and some computational aspects are discussed. Results are presented for cutoff behavior as well as general dispersion characteristics for two and three layered plates.**

I. Introduction

EXACT analysis of the propagation of acoustic waves in multilayered piezoelectric plates is performed using a general and powerful transfer matrix approach. The transfer matrix method is a very simple technique for analyzing wave phenomena in layered media. This technique, as applied to piezoelectric crystals, has its roots in the one dimensional transmission line equivalent circuit approach originally used by electrical engineers to analyze stacked crystal filters. The most general analysis of this type was given by Ballato, Bertoni, and Tamir [2]. The transfer matrix method is simply the physical equivalent of the transmission line analysis, relying on the principles of mechanics, rather than on electric circuit analysis. Adler [3] has proposed a general method for constructing transfer matrices for both bulk and surface wave problems which is based on linear systems analysis. Nowotny, Benes, and Schmid [4] developed a general one dimensional transfer matrix method for calculating the admittance matrix for stacked piezoelectric layers with arbitrary electrode placement, and Nayfeh [5] used a transfer matrix approach to solve two dimensional problems of wave propagation at arbitrary angles in multilayered nonpiezoelectric plates with monoclinic (or higher) symmetry. The present study represents a general one and two dimensional analysis of layered piezoelectric plates with general anisotropy. The one dimensional analysis presented is similar to the discussion of [4] with extensions to include lateral field excitation as well as a simplified technique for handling the effects of thin conducting electrodes on the plate's free surfaces. The two dimensional analysis presented represents, in principle, an extension of [5] to the more general case of piezoelectric layers. The two dimensional analysis is carried out for the cases of both open and short circuit conditions on the plate's free surfaces.

By definition, a transfer matrix is a linear transformation that maps a specified vector of field quantities from one point to another in a given material. When applied to a layered plate, this method greatly simplifies the analysis by guaranteeing continuity of field quantities across layer interfaces while reducing the problem to one involving these quantities evaluated at the plate's free surfaces only. More specifically, a transfer matrix for each layer is developed which maps displacements, stress tractions, electric potential, and electric charge from the layers lower surface to it's upper surface. Satisfaction of inter-layer continuity of these field quantities leads to a simple matrix multiplication rule, from which follows a global plate transfer matrix. The plate transfer matrix equation that results is represented in terms of the field quantities evaluated on the plate's free surfaces only. From this, many problems involving thickness field excitation of layered piezoelectric resonators may be handled quite readily. It is shown that, with some modifications, this method can handle problems involving lateral field excitation as well. A simple technique for incorporating the mechanical effects of thin conducting electrodes on the plates top and bottom surfaces is also presented.

The present study involves the application of the transfer matrix method to the exact analysis of simple thickness modes and general dispersion behavior in zinc oxide on Silicon thin film resonators. Fundamental resonant and antiresonant cutoff frequencies through both thickness and lateral field excitation are calculated for two and three layered plates. Along with these frequencies, thickness mode shapes for displacements, stress tractions, electric potential, and electric displacement are shown. Exact dispersion relations for propagating straight crested waves are also presented for these plates. Both real and imaginary branches of these dispersion relations are shown and these calculations are carried out for both open circuit and short circuit conditions. Two different crystal tensor rotations of the ZnO layers are considered, giving rise to different cases of electro-mechanical coupling.

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II. General Problem

Consider a plate of thickness $2b$ constructed of N anisotropic piezoelectric layers stacked normal to the x_2

A Perturbation Method for Finite Element Modeling of Piezoelectric Vibrations in Quartz Plate Resonators

Y.-K. Yong, *Member, IEEE*, and Zhen Zhang

Abstract—When the piezoelectric stiffening matrix is added to the mechanical stiffness matrix of a finite element model, its sparse matrix structure is destroyed. A direct consequence of this loss in sparseness is the significant rise in memory and computational time requirements for the model. For weakly coupled piezoelectric materials, the matrix sparseness can be retained by a perturbation method which separates the mechanical eigenvalue solution from its piezoelectric effects. A perturbation and finite element scheme for weakly coupled piezoelectric vibrations in quartz plate resonators has been developed. Finite element matrix equations were derived specifically for third overtone thickness shear, SC-cut quartz plate resonators with electrode platings. High frequency, piezoelectric plate equations, previously derived by Lee, Syngellakis, and Hou [1], were employed in the formulation of the finite element matrix equation. The equations may be used for modeling third harmonic overtone of thickness shear vibrations. Results from the perturbation method for SC-cut quartz plates compared well with the direct solution of the piezoelectric finite element equations. This method will result in significant savings in computer memory and computational time. Resonance and anti-resonance frequencies of a certain mode could be calculated easily by using the same eigen-pair from the purely mechanical stiffness matrix. Numerical results for straight crested waves in a third overtone SC-cut quartz strip with and without electrodes are presented. The steady-state response to an electrical excitation is calculated. The accuracy of the perturbation method is dependent on the magnitude of piezoelectric coupling constant in the mode of vibration. For example, an investigation on the first few modes of vibration in a cube made of lithium niobate, which has high piezoelectric coupling constants, yielded divergent results for the perturbation method. Hence, the method should not be used for materials with high piezoelectric coupling constants.

I. Introduction

We discuss in this paper a perturbation method for weakly coupled piezoelectric vibrations, the finite element formulation, and results on straight crested waves in the vicinity of a third harmonic overtone of thickness shear mode in a SC-cut quartz strip.

The straight crested waves are spatially one dimensional, but since the study is part of a wider study of third overtone SC-cut quartz resonators, two-dimensional finite element equations for piezoelectric plate vibrations are derived and presented. A one-dimensional finite element program is developed which could be modified subsequently to handle two-dimensional problems. The mechanical stiffness of the finite element matrix equations for the SC-cut quartz is a few orders of magnitude larger than the piezoelectric stiffness, hence, the piezoelectric coupling is weak, and the piezoelectric effects could be modeled using a perturbation method. A new perturbation method for piezoelectric vibrations is derived and proposed. Results for the perturbation method, free vibrations, and steady-state vibrations of a partially electroded SC-cut strip are shown.

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II. Plate Equations for High Frequency Piezoelectric Vibrations

The piezoelectric plate equations for high frequency vibrations employed in the current finite element formulation were derived by Lee, Syngellakis, and Hou [1]. The components of mechanical displacement and electric potential are expanded in an infinite series with their thickness-dependence expressed by trigonometric functions:

$$u_i(x_1,x_2,x_3,t) = \sum_{n=0}^{\infty} u_i^{(n)}(x_1,x_3,t) \cdot \cos\frac{n\pi}{2}(1-\xi) \tag{1a}$$

$$\phi(x_1,x_2,x_3,t) = \sum_{n=0}^{\infty} \phi^{(n)}(x_1,x_3,t) \cdot \cos\frac{n\pi}{2}(1-\xi) \tag{1b}$$

where $\xi = x_2/b$ is a nondimensional thickness coordinate of the plate. The terms $u_j^{(n)}$ and $\phi^{(n)}$ are functions of spatial coordinates x_1 and x_3 only, and time t. We present without formal derivations the following field equations from [1]. The interested reader may obtain details of their derivations from the same reference. Some equations are given in a matrix form to facilitate the development of finite element matrix equations.

A. Stress Equations of Motion

$$T_{ij,i}^{(n)} - \frac{n\pi}{2b}\overline{T}_{2j}^{(n)} + \frac{1}{b}F_j^{(n)} = (1+\delta_{n0})\rho\ddot{u}_j^{(n)} \tag{2a}$$

where the terms T_{ij} and $\overline{T}_{2j}$ are n-th order stresses and are defined as the following:

$$T_{ij}^{(n)} = \int_{-1}^{1} T_{ij}\cos\left[\frac{n\pi}{2}(1-\xi)\right]d\xi \tag{2b}$$

$$\overline{T}_{2j}^{(n)} = \int_{-1}^{1} T_{2j}\sin\left[\frac{n\pi}{2}(1-\xi)\right]d\xi \tag{2c}$$

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A laminated plate theory for high frequency, piezoelectric thin-film resonators

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A high frequency, piezoelectric, laminated plate theory is developed and presented for the purpose of modeling and analyzing piezoelectric thin-film resonators and filters. The laminated plate equations are extensions of anisotropic composite plate theories to include piezoelectric effects and capabilities for modeling harmonic overtones of thickness-shear vibrations. Two-dimensional equations of motion for piezoelectric laminates were deduced from the three-dimensional equations of linear piezoelectricity by expanding the mechanical displacements and electric potential in a series of trigonometric function, and obtaining stress resultants by integrating through the plate thickness. Relations for handling the mechanical and electrical effects of platings on the top and bottom surfaces of the laminate are derived. A new matrix method of correcting the cutoff frequencies is presented. This matrix method could also be used to efficiently correct the cutoff frequencies of any nth order plate laminate theories which employ Mindlin's form of polynomial expansion of mechanical displacements and electric potential through the plate thickness. The first order laminated plate theory with correction factors for cutoff frequencies and slope of the flexural branch at large frequencies was applied to a 2-layer, zinc oxide-silicon strip, and a 3-layer, zinc oxide-zinc oxide-silicon strip. Open circuit, dispersion relations were generated for a range of volume fractions and compared to the exact dispersion relations. Both the 2-layer and 3-layer strip show similar qualitative comparison: The present theory compares fairly well with the exact dispersion relation for real wave numbers and nonpropagating (imaginary) wave numbers which are smaller than $0.5i$. The extensional branch, and thickness-shear branches begin to deviate from the exact solution when the nondimensionalized frequency is greater than one. Consequently, to maintain accuracy of solutions when using the present first order laminated plate theory, one should limit the calculation of resonant, nondimensionalized frequencies to less than 1.1. Results for the frequency spectrum in the vicinity of the open circuit, fundamental thickness-shear frequency, and modes shapes were presented for the 2-layer strip with fixed edges, and a volume fraction of silicon equal to 0.2. The technically important fundamental thickness-shear mode is found to have the shear component strongly coupled with extensional component.

I. INTRODUCTION

We discuss in this paper the development and application of a high frequency piezoelectric, laminated plate theory intended for analyzing and modeling piezoelectric thin-film resonators. An overall view of the thin-film resonator technology is given in Refs. 1 and 2. The resonator itself is also referred to by other names such as bulk wave composite resonator[3] and film bulk acoustic resonator.[2] Theoretical analysis and modeling of the thin-film resonator was restricted to simple one-dimensional models until Milsom's[3] two-dimensional analysis of a thickness-extensional mode resonator employing zinc oxide thin films on silicon; and later, Tiersten and Stevens's[4] analysis of a thickness-extensional trapped energy resonator with rectangular electrodes in a similar device. Piezoelectric plate theories for low frequency flexural and torsional vibrations of piezoelectric, laminated polymer plates were studied by Ricketts[5] and Lee and Moon.[6]

The thin-film resonators of interest are excited at high frequencies in the vicinity of the fundamental thickness modes and their higher harmonic overtones. The analysis of such modes of vibrations would require either a three-dimensional theory, or a high frequency, piezoelectric, laminated plate theory. One could argue that a piezoelectric composite could always be modeled using three-dimensional finite elements such as those presented by Allik and Hughes[7] and Lerch.[8] There exist commercial finite element software packages which have a three-dimensional piezoelectric element. Such a route for high frequency problems is extremely intensive in terms of memory requirements and numerical computations. The difficulty in identifying the resonant frequency of interest and its mode shape increases rapidly with the frequency of vibration. The problem becomes quite intractable for higher harmonic overtones of thickness-shear vibrations. A high frequency plate theory would, besides being less intensive in terms of memory requirements and numerical computations, alleviate part of this problem because the displacements through the plate thickness are assumed known and are expressed in a fixed number of displacement components $u_i^{(n)}$. Hence, other than its theoretical complexities

ALGORITHMS FOR EIGENVALUE PROBLEMS IN PIEZOELECTRIC FINITE ELEMENT ANALYSES

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ABSTRACT

Two algorithms for eigenvalue problems in piezoelectric finite element analyses are introduced. The first algorithm involves the use a Lanczos eigensolver, while the second algorithm uses a Rayleigh quotient iteration scheme. In both solution methods, schemes are implemented to reduce storage requirements and solution time. Also, both solution methods seek to preserve the sparsity structure of the stiffness matrix to realize major savings in memory. In the Lanczos solution method, the structural pattern of the consistent mass matrix is exploited to gain savings in both memory and solution time. In the Rayleigh quotient iteration method, an algorithm for generating good initial eigenpairs is employed to improve significantly its overall convergence rate, and convergence stability in the regions of closely spaced eigenvalues and repeated eigenvalues. The initial eigenvectors are obtained by interpolation from a coarse mesh. In order for this iterative method to be effective, an eigenvector of interest in the fine mesh must resemble an eigenvector in the coarse mesh. Hence, the method is effective for finding the set of eigenpairs in the low frequency range, and not in the high frequency range where the eigenvectors of the coarse mesh does not resemble well their counterparts in the fine mesh. Results of example problems are presented to show the savings in solution time and storage requirements of the proposed algorithms when compared with the conventional algorithm which uses static condensation to remove the electric potential degrees of freedom from the piezoelectric eigenvalue problem. The disadvantage of this conventional scheme is that the static condensation destroys the sparsity structure of the stiffness matrix, which leads to major increases in memory and solution time.

INTRODUCTION

The analysis and design of piezoelectric resonator devices present a challenging set of attributes to the engineer: (1) The geometry and boundary conditions of the devices are complex, (2) the resonating element is a composite, consisting of metal electrodes on a piezoelectric plate or substrate, and in thin film devices, the piezoelectric layer is grown on a dielectric layer, and (3) the devices usually operate at higher modes vibrations. Hence, the analysis of these devices demands good analytical models, and detailed finite element solution of such analytical models. This is especially relevant when accurate prediction of the unwanted modes is required.

The numerical models would generate a set of coupled piezoelectric eigenvalue equations of the following form:

$$M\ddot{u} + K_{uu}u + K_{u\phi}\phi = F, \tag{1}$$

$$K_{\phi u}u + K_{\phi\phi}\phi = Q \tag{2}$$

where the matrices M, K_{uu}, $K_{u\phi}$ and $K_{\phi\phi}$ are the mass, mechanical stiffness, piezoelectric coupling, and dielectric matrices respectively. The vectors u, ϕ, F and Q are respectively the mechanical displacement, electric potential, mechanical force and electric charge vectors. A static condensation[1] of the potential ϕ in eqs. (1) and (2) renders a single equation written as

$$M\ddot{u} + K^*u = F^*, \tag{3}$$

where

$$K^* = K_{uu} - K_{u\phi}K_{\phi\phi}^{-1}K_{\phi u} \tag{4}$$

and

$$F^* = F - K_{u\phi}K_{\phi\phi}^{-1}Q. \tag{5}$$

K^* is the condensed electroelastic stiffness matrix and F^* is the corresponding electromechanical forcing function. The components of the electric potential vectors are recovered from eq. (2) by

$$\phi = K_{\phi\phi}^{-1}(Q - K_{\phi u}u). \tag{6}$$

A generalized eigenvalue problem can be obtained from eq. (3) by assuming harmonic solutions, and setting F^* equal to zero to yield

$$(K^* - \omega^2 M)u = 0, \tag{7}$$

where ω is the natural frequency.

Abstract Of The Dissertation

Exact And Approximate Analysis Of The Propagation Of Acoustic Waves In Layered Piezoelectric Plates

by James T. Stewart

Dissertation Director:

Professor Yook-Kong Yong

Exact and approximate analysis of the propagation of acoustic waves in layered piezoelectric plates is performed with specific application to the analysis of thin film resonators. The exact analysis is performed using the transfer matrix method. By definition, a transfer matrix is a linear transformation which maps a specified vector of field quantities from one point to another in a material. By constructing transfer matrices for each layer and enforcing inter-layer continuity of pertinent field quantities, a simple matrix multiplication rule results which can be used to map these quantities from the plate's lower free surface to its upper free surface. The result is a problem which is in terms of the field quantities evaluated on the plate's free surfaces only, which is no more difficult to solve than it is for a homogeneous plate. The transfer matrix analysis is directly applicable to problems of thickness excitation and it will be shown that, with some modifications, this method can be used to study problems of lateral excitation. The approximate analysis is performed using a high frequency laminate theory. The laminated plate equations are developed using two different series expansions for the thickness dependency of displacements and electric potential. A general correction method is developed which improves the accuracy of the approximate solutions. In the first analysis, a power series expansion is used, and later a trigonometric series expansion is applied. Cutoff behavior as well as general dispersion characteristics for Zinc Oxide on Silicon thin film resonators are studied using the approximate analysis and compared to the exact solutions. In the final analysis, a layered piezoelectric strip of finite length is studied under conditions of free vibration with mechanically clamped ends.

ABSTRACT OF THE DISSERTATION

Numerical Analysis of The Third Overtone of Thickness Shear Vibrations in SC-cut Quartz Resonators

by Zhen Zhang , Ph.D.

Dissertation Director: Professor Yook-kong Yong

Exact and approximate dispersion relations up to the third overtone of thickness shear are developed for an infinite SC-cut quartz piezoelectric plate with the triclinic symmetry (all 36 quantities are present in the elastic tensor) using the three-dimensional piezoelectricity and a two-dimensional piezoelectric, high frequency plate theory, respectively. By comparing the results, the approximate theory is found to provide an excellent approximation of the vibrational behavior of SC-cut quartz plate resonators.

A realistic and detailed finite element model of piezoelectric plate resonators, which takes into consideration of the effects of the electrodes, is developed. The finite element formulation is derived based on the general N-th order plate equations using the variational principle. The finite element matrix equations from the third order

plate equations are used in the analysis of the third overtone of thickness shear. The finite element model developed in this work may be employed in high frequency SC-cut quartz plate resonator analysis to obtain characteristics of vibration such as resonant frequencies and mode shapes which would otherwise be available experimentally through elaborate and costly laboratory work.

Numerical strategies for solving very large scale finite element model of SC-cut quartz resonators are explored. A perturbation technique is developed to account for the piezoelectric effect for weakly coupled material. This method saves substantial memory and computational time, and is found to be rather accurate for SC-cut quartz. In the calculations of the purely mechanical eigenpairs, a new storage scheme for the mass matrix is proposed. The scheme makes use of the special structure of the mass matrix and reduces the memory requirement by more than 90% over that of the envelope storage scheme in the current analysis. The substructuring technique is introduced into the eigenvalue calculations to further diminish the memory demands as well as the computational time without any loss of accuracy.

Numerical analysis of the third overtone of thickness shear of SC-cut quartz resonators is performed using the finite element method. Frequency spectra, resonant frequencies and mode shapes are calculated and presented. Vibrational characteristics of the predominant mode is studied with the effects of the electrodes.